Ising spin glass transition in magnetic field out of mean-field

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The spin-glass transition in external magnetic field is studied both in and out of the limit of validity of mean-field theory on a diluted one dimensional chain of Ising spins where exchange bonds occur with a probability decaying as the inverse power of the distance. Varying the power in this long-range model corresponds, in a one-to-one relationship, to change the dimension in spin-glass short-range models. Evidence for a spin-glass transition in magnetic field is found also for systems whose equivalent dimension is below the upper critical dimension at zero magnetic field.

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Introduction – Even though 30 years have passed since the spin-glass (SG) phase in presence of an external magnetic field has been characterized in mean-field theory [1], its existence in realistic finite-dimensional systems is not yet an established issue. In most common (Heisenberg-like) amorphous magnets, e.g., AgMn, CuMn, and AuFe, a SG phase has been detected also in presence of an external field [2]. In mean-field theory of vectorial spin-glasses this transition is expected along the so-called Gabay-Toulouse line [3]. In Ising-like materials, instead, like $Fe_xMn_{1-x}TiO_3$, it is still a matter of debate whether or not a SG phase occurs when the system is embedded in a magnetic field [2, 4]. Irreversible phenomena are, actually, detected in experiments as the temperature is lowered: the separation of zero-field cooled and field-cooled susceptibilities (or magnetizations) and the rapid increase of characteristic relaxation times. In zero field these are the signatures of a thermodynamic transition, but in some recent AC measurements in a magnetic field [4], their magnitude tends to depend sensitively on frequency and they are interpreted as pertaining to a glassy dynamic arrest, rather than to a true thermodynamic transition. According to this, the SG features measured in a field would be artifacts of being out of equilibrium, similarly to what happens in the structural glass transition, in which the liquid glass former falls out of equilibrium at some low T when its structural relaxation time becomes longer than the observation time and it vitrifies into an amorphous solid.

The Replica Symmetry Breaking (RSB) theory, holding in the mean-field regime for spin-glasses, predicts a thermodynamic transition in magnetic field h at a finite temperature [5]. In this framework, a transition line, called Almeida-Thouless (AT) [1] line, can be identified in the $T-h$ plane between a paramagnetic and a spin glass phase. At sufficiently low dimensions (i.e. below the lower critical dimension, $D_{\rm L}$) the transition disappears. The value of $D_{\rm L}$ is not known, but it is quite possible that in a field $D_{\rm L}$ is higher than for $h=0$ (as it happens for a ferromagnet in a random field). There are some numerical evidences (and analytic results) supporting $D_{\rm L}$= 2.5 at zero field. For $h>0$, some arguments suggested $D_{\rm L}$=6, but recently Temesvari [6] argued that the AT line can be continued below $D=6$. In the droplet theory, instead, no transition is predicted to remain as soon as an infinitesimal field is switched on, independently from the value of D. A crossover length $\ell_d(h,T)$ is introduced [7], beyond which the SG phase is destroyed by the field. The predictions of TNT scenario [8] should be similar to those of the droplet model. Extensive numerical works on the Edwards-Anderson model in 4D and 3D yielded evidence both in favor of a transition in field [9, 10] and against it [11, 12, 13]. Unfortunately, finite size corrections are very strong in the presence of an external field and it is hard to say whether these simulations were really testing the thermodynamic limit. To overcome this problem we use a recently introduced SG model [14], which can be simulated very efficiently, and a new data analysis, which should be less sensitive to finite size effects. We report numerical evidences for a thermodynamic phase transition in the presence of external fields also in systems for which the mean-field approximation is not correct.

The model – We investigate a one dimensional chain of L Ising spins ($\sigma_i=\pm 1$) whose Hamiltonian reads [14]

$$\mathcal{H} = -\sum_{i<j} J_{ij}\sigma_i\sigma_j - \sum_i h_i\sigma_i \ . \qquad (1)$$

The quenched random couplings J_{ij} are independent and identically distributed random variables taking a non zero value with a probability decaying with the distance between spins σ_i and σ_j, $r_{ij}\equiv \min(|i-j|, L-|i-j|)$, as

$$\mathbf{P}[J_{ij}\neq 0] \propto r_{ij}^{-\rho} \quad \text{for} \ \ r_{ij}\gg 1 \ . \qquad (2)$$

Non-zero couplings take value ± 1 with equal probability. We use periodic boundary conditions and a $z=6$ average coordination number [23]. The random field h_i is Gaussian distributed with zero average and standard deviation h [24]. We will denote the average over quenched disorder, both bonds and fields, by an overline. The universality class depends on the value of ρ. For $\rho>1$ it

turns out to be equal to the one of the fully connected version of the model [15], where bonds are Gaussian distributed with zero mean and a variance depending on the distance as $\overline{J_{ij}^2} \propto r_{ij}^{-\rho}$. As ρ varies, the model displays different behaviors [14]: for $\rho \leq \rho_U \equiv 4/3$, the mean-field (MF) approximation is exact, while for $\rho > \rho_U$, it breaks down because of infrared divergences (IRD). The value $\rho_{\rm U} = 4/3$ corresponds to the upper critical dimension of short-range spin-glasses in absence of an external magnetic field ($D_{\rm U} = 6$). At $\rho > \rho_{\rm L} = 2$ no finite temperature transition occurs, even for $h = 0$ [16]. A relationship between ρ and the dimension D of short-range models can be expressed as $\rho = 1 + 2/D$ which is exact at $D_{\rm U} = 6$ ($\rho_{\rm U} = 4/3$) and approximated as $D < D_{\rm U}$. Indeed, the lower critical dimension $D_{\rm L} \simeq 2.5$ [17] corresponds to $\rho \simeq 1.8$, which is 10% less than $\rho_{\rm L}$. We note that in the ferromagnetic (ordered) Ising case on the same kind of lattices a simple theoretical argument tells us that the value of $\rho_{\rm L}$ is 2 for $h = 0$ and 1.5 in a field.

Simulations details and data analysis – To study the critical behavior of the model in external field we simulated two replicas $\sigma_i^{(1,2)}$ using the parallel tempering (PT) algorithm [18]. Field values are $h = 0, 0.1, 0.2, 0.3$ for $\rho = 0, 1.2, 1.4$ and $h = 0, 0.1, 0.15$ for $\rho = 1.5$. We used sizes up to $L = 2^{14}$ spins for $h = 0$ and up to $L = 2^{12}$ for $h > 0$. The number of samples is between 32000 and 64000 for all sizes. Thermalization is guaranteed by the logarithmic binning (in base 2) of data in MC steps until at least the last two points coincide. The presence of SG long range order can be deduced from the study of the four-point correlation function

$$C(x) = \sum_{i=1}^{L} \overline{\left(\langle \sigma_i \sigma_{i+x} \rangle - \langle \sigma_i \rangle \langle \sigma_{i+x} \rangle\right)^2} \qquad (3)$$

and its Fourier transform $\widetilde{C}(k)$ [25]. Indeed, both the SG susceptibility

$$\chi_{\rm sg} \equiv \widetilde{C}(0) \qquad (4)$$

and the so-called second-moment correlation length [19]

$$\xi \equiv \frac{1}{2\sin(\pi/L)} \left[\frac{\widetilde{C}(0)}{\widetilde{C}(2\pi/L)} - 1 \right]^{\frac{1}{\rho-1}} \qquad (5)$$

diverge at the critical temperature in the thermodynamic limit. For finite (but large enough) systems, the following scaling laws hold in the MF regime ($1 < \rho \leq 4/3$)

$$\frac{\chi_{\rm sg}}{L^{1/3}} = \tilde{\chi}\left(L^{\frac{1}{3}}(T - T_c)\right), \quad \frac{\xi}{L^{\nu/3}} = \tilde{\xi}\left(L^{\frac{1}{3}}(T - T_c)\right) \quad (6)$$

with $\nu = 1/(\rho - 1)$, and in the IRD regime ($\rho > 4/3$)

$$\frac{\chi_{\rm sg}}{L^{2-\eta}} = \tilde{\chi}\left(L^{\frac{1}{\nu}}(T - T_c)\right), \quad \frac{\xi}{L} = \tilde{\xi}\left(L^{\frac{1}{\nu}}(T - T_c)\right). \quad (7)$$

with $2 - \eta = \rho - 1$. Unfortunately finite size corrections to the above scaling laws are known to be very large, especially in the presence of an external field. It is very important to understand these finite size effects (FSE) and try to keep them under control.

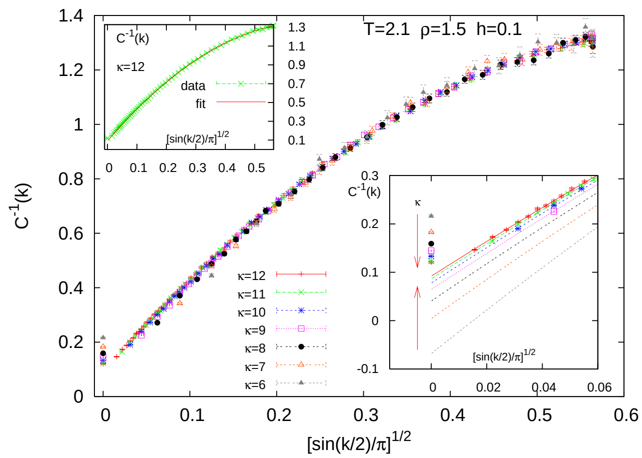

FIG. 1: $\widetilde{C}(k)^{-1}$ vs. $\sqrt{\sin(k/2)/\pi}$ at $\rho = 1.5$ (IRD regime), $h = 0.1$, $T = 2.1$ and $L = 2^\kappa$, with $\kappa = 6, \ldots, 12$. Upper inset: quadratic fit to $L = 2^{12}$ data, excluding $k = 0$. Lower inset: comparison between $\widetilde{C}(0)^{-1}$ and its extrapolated valued A.

In the main panel of Fig. 1 we plot $1/\widetilde{C}(k)$ versus $[\sin(k/2)/\pi]^{\rho-1}$ for an interesting case (IRD regime with field). The choice of the variables is dictated by the fact that for $L \to \infty$ and $T > T_c$ the propagator on the lattice at small wave numbers should behave like

$$\widetilde{C}(k)^{-1} \simeq A + B[\sin(k/2)]^{\rho-1}, \qquad (8)$$

with $\chi_{\rm sg} = 1/A$ and $\xi \propto (B/A)^{1/(\rho-1)} = (B\chi_{\rm sg})^{1/(\rho-1)}$. In other words, $A(L = \infty, T)$ goes to zero at T_c, while $B(L = \infty, T = T_c)$ stays finite.

We observe in Fig. 1 that the largest FSE in $\widetilde{C}(k)$ are in $k = 0$, which is the data used for estimating $\chi_{\rm sg}$. Moreover FSE for $k > 0$ have an opposite sign with respect to those in $k = 0$ (cf. lower inset) and consequently ξ, which is a function of $\widetilde{C}(0)/\widetilde{C}(2\pi/L)$, may be strongly affected. The reason why FSE become smaller increasing k is simple: they are more evident in the large x tail of $C(x)$ and, thus, at small k in $\widetilde{C}(k)$. Moreover, the large x part of $C(x)$ strongly depends on $\overline{\langle q \rangle}$, which is known to have large sample-to-sample fluctuations in a field and FSE due to negative overlaps which should disappear in the thermodynamic limit.

With the aim of reducing FSE, we introduce a method for estimating T_c using $\widetilde{C}(k)$ data with $k > 0$. We fit $\widetilde{C}(k)^{-1}$ by a quadratic function $A + By + Cy^2$ with $y = [\sin(k/2)/\pi]^{\rho-1}$: the goodness of such a fit can be appreciated in the upper inset of Fig. 1. As long as $T > T_c$, we expect $\lim_{L\to\infty} A(L,T) = \chi_{\rm sg}^{-1} > 0$: the lower inset in Fig. 1 shows size dependence of $\widetilde{C}(0)^{-1}$ and $A(L,T)$, having compatible thermodynamic limits.

In the main panel of Fig. 2 we show the best fitting

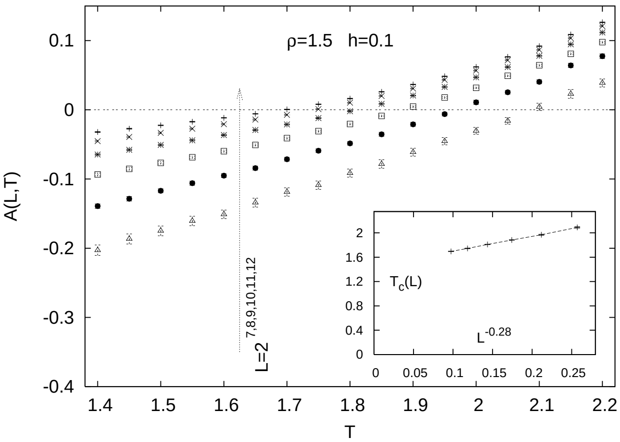

FIG. 2: Plot of $A(L,T)$ vs. T at $\rho = 1.5$, $h = 0.1$. Sizes are $L = 2^{\kappa}$, with $\kappa = 7, \ldots, 12$. Inset: $T_c(L)$ vs. $L^{-0.28}$.

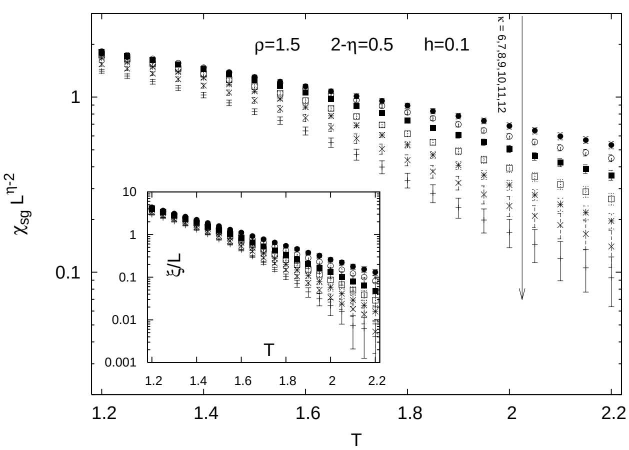

FIG. 3: Plot of $\chi_{\rm sg}/L^{0.5}$ vs. T at $\rho = 1.5$, $h = 0.1$. Sizes are $L = 2^{\kappa}$, with $\kappa = 6, \ldots, 12$. Inset: ξ/L vs. T.

parameter $A(L,T)$ for $\rho = 1.5$ and $h = 0.1$. For each size we compute the temperature $T_c(L)$ by solving the equation $A(L, T_c(L)) = 0$ (in this way only $A > 0$ data are used, which are the most reliable). Finally, we estimate $T_c = \lim_{L\to\infty} T_c(L)$ (inset of Fig. 2) and obtain $T_c = 1.46(3)$. The $T_c(L)$ scaling in $L^{-1/\nu}$ has an exponent -0.28, in good agreement with $1/\nu = 0.25(3)$ for the $h = 0$ case [14]. On the same data ($\rho = 1.5$, $h = 0.1$) the analysis of the crossing points of $\chi_{\rm sg}/L^{2-\eta}$ and ξ/L, cf. Eq. (7), is shown in Fig. 3, yielding no evidence for a phase transition. The most natural explanation is the presence of corrections to scaling laws Eq. (7).

The case $\rho = 1.4$ and $h = 0.1$ provides a still more useful comparison. Our method of analysis returns a critical temperature $T_c = 1.67(7)$. Fig. 4 shows $\chi_{\rm sg}/L^{2-\eta}$ and ξ/L vs. T: crossings are present, but the curves seem to merge for $T \lesssim 1.5$ and a precise determination of T_c is

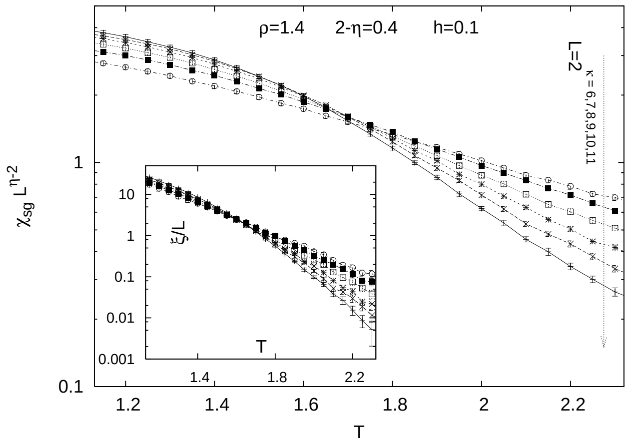

FIG. 4: Plot of $\chi_{\rm sg}/L^{0.4}$ vs. T at $\rho = 1.4$, $h = 0.1$. Sizes are $L = 2^{\kappa}$, with $\kappa = 6, \ldots, 12$. Inset: ξ/L vs. T.

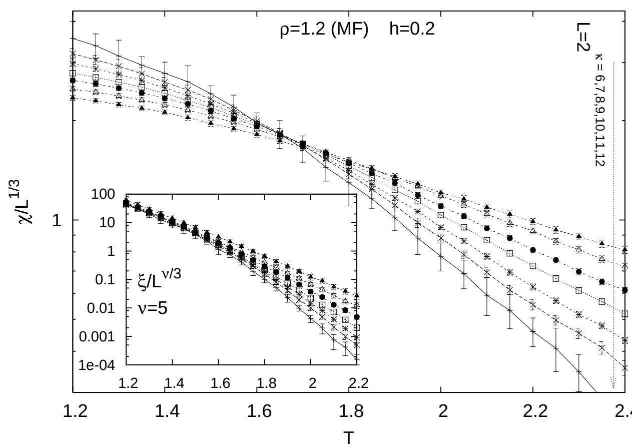

FIG. 5: Plot of $\chi_{\rm sg}/L^{1/3}$ vs. T at $\rho = 1.2$, $h = 0.2$. Sizes are $L = 2^{\kappa}$, with $\kappa = 6, \ldots, 12$. Inset: $\xi/L^{\nu/3}$ vs. T.

practically unfeasible. For $\rho = 1.2$, $h = .2$, cf. Fig. 5, the estimate based on the scaling of $\chi_{\rm sg} \sim L^{1/3}$ - Eq.(6) - yields $T_c = 1.67(3)$, while the $\xi/L^{\nu/3}$ curves do not show any crossing for $T > 1.2$. Since the transition is known to be there in MF, this behavior of ξ is clearly caused by large FSE.

Numerical values for the estimates of T_c obtained with the two methods are reported in Table I and look compatible. It is clear that for large ρ our method works better. As ρ is decreased, this new estimate becomes poorer, because the scaling exponent $\rho - 1$ [cf. Eq.(8)] is too small to yield a robust extrapolation of $A(L,T)$.

Discussion of experimental results – A possible objection to the presence of the SG transition (supported by our results) is that in experiments on Ising-like SG no AT line was detected. Here we consider, in particular, the most recent experiments on $Fe_{0.55}Mn_{0.45}TiO_3$ [4], where the AC susceptibilities were very accurately measured in

	ρ	"D"	h	T_c from $\widetilde{C}(0)$	T_c from $A(L,T)$
MF	1.2	10	0.0	2.24(1)	2.34(3)
	1.2	10	0.1	2.02(2)	1.9(2)
	1.2	10	0.2	1.67(3)	1.4(2)
	1.2	10	0.3	1.46(3)	1.5(4)
	1.25	8	0.0	2.191(5)	2.23(2)
IRD	1.4	5	0.0	1.954(3)	1.970(2)
	1.4	5	0.1	~ 1.5	1.67(7)
	1.4	5	0.2	~ 1.1	1.2(2)
	1.5	4	0.0	1.758(4)	1.770(5)
	1.5	4	0.1	—	1.46(3)
	1.5	4	0.15	—	1.20(7)

TABLE I: Estimates of T_c: column 5 from Eqs.(6–7) and column 6 from the extrapolation of $A(L,T)$ by Eq.(8).

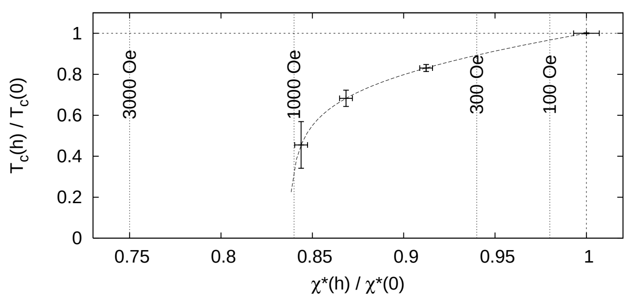

FIG. 6: Relative decrease of the critical temperature with increasing field ($\rho = 1.5$, $h = 0, 0.1, 0.15, 0.2$) versus relative decrease of χ^*, the ZFC susceptibility at $T_c(h = 0)$. The dashed curve is a guide for the eye.

the presence of an external magnetic field. In order to relate external fields in our model to those used in experiments we look how much the zero-field-cooled (ZFC) susceptibility at temperature $T_c(h = 0)$, χ^*, decreases as h is increased. In Fig. 6 we plot $T_c(h)/T_c(0)$ versus $\chi^*(h)/\chi^*(0)$ in our model for $\rho = 1.5$. In experiments on $Fe_{0.55}Mn_{0.45}TiO_3$[4] with external fields of magnitude 100 Oe, 300 Oe, 1000 Oe and 3000 Oe one has, respectively, $\chi^*(h)/\chi^*(0) = 0.98, 0.94, 0.84, 0.75$. These ratios, cf. Fig. 6, suggest that a SG transition is unlikely to be experimentally observed above $h = 1000$ Oe.

Increasing ρ, and/or considering $\overline{J_{ij}} \neq 0$, the critical field decreases. The $\rho = 1.5$ model considered above is approximately equivalent to a short-range system in $D = 4$. Therefore, in order to detect, or rule out, a SG phase in $D = 3$, it becomes even more important to work at small fields. The observation that the fields used in experiments on Ising-like materials are maybe too large to see a SG phase is in agreement with the results of Petit *et al.*, who studied both Ising-like and Heisenberg-like spin glass samples [2].

Conclusions – In conclusion, by using a new method of data analysis, we have been able to identify an AT transition line in the diluted power-law decaying interaction Ising SG chain at all values of the power analyzed, including values corresponding to short-range SG models below the upper critical dimension. The behaviour below the AT line may change with the dimension. We are presently studying this possibility.

These AT lines were not found in the study of the fully connected version performed in Ref. [21], nor in Ref. [22] where a similar diluted model was simulated [26]. There, T_c was estimated by using the scaling properties of ξ/L. As we have shown, this quantity suffers of strong FSE. We put forward an alternative method to discriminate between a pure paramagnetic phase at all temperatures and a finite temperature spin-glass transition. One of the advantages of this method is that it mainly uses data at $T > T_c$, leading to more reliable results.

For what concerns three dimensional real systems, we hint that the magnitude of the external fields used in experiments up to now might be too large to firmly rule out the presence of an AT transition line. We suggest a range of fields ($h < 1000$ Oe) where the transition should take place in $Fe_{0.55}Mn_{0.45}TiO_3$ and we hope this may stimulate further experimental investigations.

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[23] The value $z = 6$ is a compromise: the computer time is proportional to z but the critical temperature approaches zero for small z (with drawbacks in its evaluation).

[24] For these systems the effect of a random local field is very similar to a uniform one [11, 20, 21] but has some advantages in performing the numerical simulations.

[25] In our algorithm we measure directly $\widetilde{C}(k)$ and to save computing time we express $C(x)$ as linear combination of $\overline{\langle h_i h_j \sigma_i^{(1)} \sigma_j^{(2)} \rangle}$, $\overline{\langle h_i \sigma_i^{(1)} \sigma_i^{(2)} \sigma_j^{(2)} \rangle}$ and $\overline{\langle \sigma_i^{(1)} \sigma_j^{(1)} \sigma_i^{(2)} \sigma_j^{(2)} \rangle}$.

[26] Minor differences are present in that model: (i) a geometric distance in a circle, rather than a distance along the line with periodic boundary conditions, and (ii) Gaussian couplings instead of bimodal ones. These are not strongly affecting the critical behavior.